Appendix B: Residue Parameter Files

Parameter files describing the chemical and structural properties of each residue is found in the PyRosetta package in the database/chemical/residue_type_sets directory.

The full-atom residue parameters are stored in the /fa_standard/residue_types directory. As an example, the parameter file for threonine is shown below.

```
NAME THR
IO_STRING THR T
TYPE POLYMER #residue type
AA THR
ATOM  N    Nbb  NH1  -0.47
ATOM  CA   CAbb CT1  0.07
ATOM  C    CObb C    0.51
ATOM  O    OCbb O    -0.51
ATOM  CB   CH1  CT1  0.14
ATOM  OG1  OH   OH1  -0.66
ATOM  CG2  CH3  CT3  -0.27
ATOM  H    HNbb H    0.31
ATOM  HG1  Hpol H    0.43
ATOM  HA   Hapo HB   0.09
ATOM  HB   Hapo HA   0.09
ATOM 1HG2  Hapo HA   0.09
ATOM 2HG2  Hapo HA   0.09
ATOM 3HG2  Hapo HA   0.09
LOWER_CONNECT N
UPPER_CONNECT C
BOND  N    CA
BOND  N    H
BOND  CA   C
BOND  CA   CB
BOND  CA   HA
BOND  C    O
BOND  CB   OG1
BOND  CB   CG2
BOND  CB   HB
BOND  OG1  HG1
BOND  CG2 1HG2
BOND  CG2 2HG2
BOND  CG2 3HG2
CHI 1  N    CA   CB   OG1
CHI 2  CA   CB   OG1  HG1
PROTON_CHI 2 SAMPLES 3 60 -60 180 EXTRA 1 20
```

Residue identification information

PDB atom names, Rosetta atom types, and partial charges

Polymer connectivity information

Bond connectivity information

Defining side-chain torsion angles

Defining proton side-chain torsion angle sampling

```
PROPERTIES PROTEIN POLAR
NBR_ATOM CB
NBR_RADIUS 3.4473
FIRST_SIDECHAIN_ATOM CB
ACT_COORD_ATOMS OG1 END
ICOOR_INTERNAL    N      0.000000    0.000000    0.000000   N     CA    C
ICOOR_INTERNAL    CA     0.000000  180.000000    1.458001   N     CA    C
ICOOR_INTERNAL    C      0.000000   68.800049    1.523257   CA    N     C
ICOOR_INTERNAL  UPPER  149.999954   63.800026    1.328685   C     CA    N
ICOOR_INTERNAL    O    180.000000   59.199905    1.231016   C     CA  UPPER
ICOOR_INTERNAL    CB  -121.983574   68.467087    1.539922   CA    N     C
ICOOR_INTERNAL    OG1   -0.000077   70.419235    1.433545   CB    CA    N
ICOOR_INTERNAL    HG1    0.000034   70.573135    0.960297   OG1   CB    CA
ICOOR_INTERNAL    CG2 -120.544136   69.469185    1.520992   CB    CA    OG1
ICOOR_INTERNAL   1HG2 -179.978256   70.557961    1.089826   CG2   CB    CA
ICOOR_INTERNAL   2HG2  120.032188   70.525108    1.089862   CG2   CB   1HG2
ICOOR_INTERNAL   3HG2  119.987984   70.541740    1.089241   CG2   CB   2HG2
ICOOR_INTERNAL    HB  -120.292923   71.020676    1.089822   CB    CA    CG2
ICOOR_INTERNAL    HA  -120.513664   70.221680    1.090258   CA    N     CB
ICOOR_INTERNAL  LOWER -149.999969   58.300030    1.328684   N     CA    C
ICOOR_INTERNAL    H    180.000000   60.849979    1.010000   N     CA  LOWER
```

Residue properties

Defining parameters for neighbor calculations

Residue structure defined in internal coordinates

The centroid residue parameters can be found in the /centroid/residue_types directory. The centroid parameter file for Threonine is shown below.

```
NAME THR
IO_STRING THR T
TYPE POLYMER #residue type
AA THR
ATOM  N   Nbb  NH1  -0.47
ATOM  CA  CAbb CT1  0.07
ATOM  C   CObb C    0.51
ATOM  O   OCbb O    -0.51
ATOM  CB  CB    CT1  0.14
ATOM  H   HNbb H    0.31
LOWER_CONNECT N
UPPER_CONNECT C
BOND  N    CA
BOND  N    H
BOND  CA   C
BOND  CA   CB
BOND  C    O
PROPERTIES PROTEIN POLAR
NBR_ATOM CEN
NBR_RADIUS 3.025
FIRST_SIDECHAIN_ATOM CB
ICOOR_INTERNAL    N      0.000000    0.000000    0.000000   N     CA    C
ICOOR_INTERNAL    CA     0.000000  180.000000    1.458001   N     CA    C
ICOOR_INTERNAL    C      0.000000   68.800049    1.523257   CA    N     C
ICOOR_INTERNAL  UPPER  149.999954   63.800026    1.328685   C     CA    N
ICOOR_INTERNAL    O    180.000000   59.199905    1.231016   C     CA  UPPER
ICOOR_INTERNAL    CB  -121.983574   68.467087    1.539922   CA    N     C
ICOOR_INTERNAL  LOWER -149.999969   58.300030    1.328684   N     CA    C
ICOOR_INTERNAL    H    180.000000   60.849979    1.010000   N     CA  LOWER
##centroid-specific
ATOM  CEN CEN_THR H 0.(
BOND CA CEN
ICOOR_INTERNAL    CEN -128.951279   72.516479    2.072556    CA     N     C
```

Residue identification information

PDB atom names, Rosetta atom types, and partial charges

Polymer connectivity information

Bond connectivity information

Residue properties

Defining parameters for neighbor calculations

Residue structure defined in internal coordinates

Centroid-specific information